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2-(Naphthalen-1-yl)ethanol

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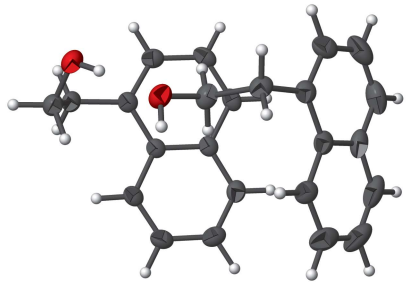
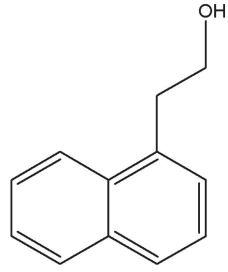
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{12}H_{11}OH$, crystallizes with two molecules, *A* and *B*, in the asymmetric unit with different conformations of the ethanol side chain; one is *gauche* [torsion angle = 59.58 (17)°] and the other is *anti* [176.20 (13)°]. In the crystal, [100] chains of alternating *A* and *B* molecules are linked by O—H···O hydrogen bonds.

3D view



Chemical scheme



Structure description

The title compound was synthesized by selective hydrogenation of the corresponding ester $C_{10}H_7CH_2CH_2CO_2Et$ (Adkins & Burgoyne, 1949) and has some applications as a synthetic block (Huang *et al.*, 2014) and as a labeling agent. One of applications is detection of low concentrations of oxygen-containing functional groups through fluorescent labeling (Feng *et al.*, 2006).

The title compound crystallizes with two molecules in the asymmetric uint: both molecules exhibit standard bond lengths and angles and almost planar naphthalene rings (Fig. 1). They differ in the conformations of the ethanol side-chains; the C1—C11—C12—O1 torsion angle of 176.20 (13)° indicates an anti orientation, whereas the equivalent angle in the second molecule [C21—C31—C32—O2 = 59.58 (17)°] corresponds to a *gauche* conformation. In the crystal, chains of alternating C1- and C21-molecules are linked by O—H···O hydrogen bonds (Table 1, Fig. 2), generating *C*(2) [100] chains.

Synthesis and crystallization

The title compound is commercially available from Aldrich as 1-napthaleneethanol. The bulk material is suitable for X-ray structure determination (Fig. 3); re-crystallization from acetonitrile yields better quality crystals which were used in current study.

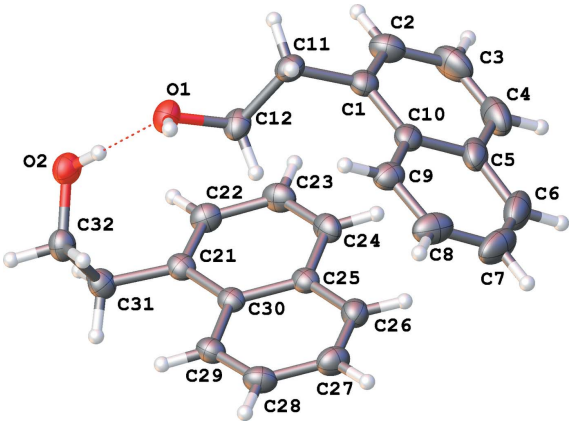


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. An intramolecular hydrogen bond is shown as a dashed line.

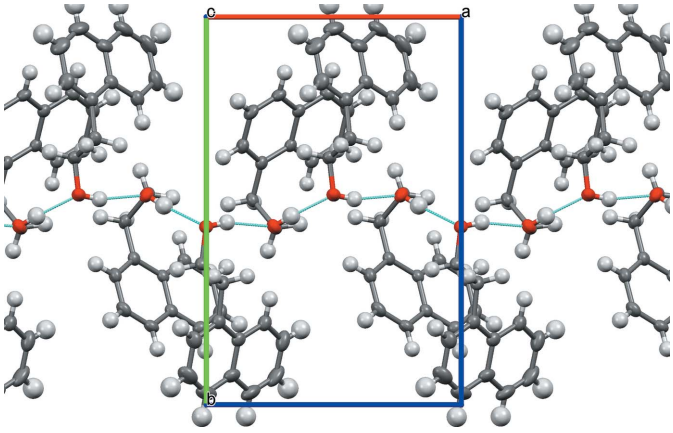


Figure 2
An infinitive chain of 2-(naphthalen-1-yl)ethanol molecules connected *via* hydrogen bonds. The view is along the *c* axis. Hydrogen bonds are shown as dashed lines.

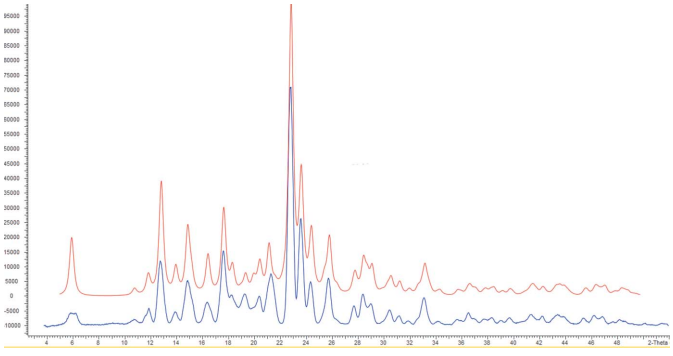


Figure 3
X-ray powder diffraction diagram of polycrystalline 2-(naphthalen-1-yl)ethanol. Blue line: experimental data after baseline correction. Red line: Simulation from single-crystal data (this structure).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.86 (3)	1.96 (3)	2.7931 (17)	163 (2)
O2—H2A···O1	0.84 (3)	1.94 (3)	2.7834 (17)	176 (2)

Symmetry code: (i) $x+\frac{1}{2}, -y+1, z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{12}H_{12}O$
M_r	172.22
Crystal system, space group	Orthorhombic, $Pca2_1$
Temperature (K)	173
a, b, c (Å)	9.8022 (6), 14.9047 (9), 12.6430 (7)
V (Å^3)	1847.13 (19)
Z	8
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.60
Crystal size (mm)	0.59 × 0.44 × 0.22
Data collection	
Diffractometer	Bruker PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.776, 0.931
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	60021, 3937, 3893
R_{int}	0.024
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.636
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.028, 0.074, 1.04
No. of reflections	3937
No. of parameters	261
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.14, −0.16
Absolute structure	Flack x determined using 1786 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.04 (3)

Computer programs: *APEX2* (Bruker, 2013), *SAINT* (Bruker, 2013), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009).

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x160423 [doi:10.1107/S2414314616004235]

2-(Naphthalen-1-yl)ethanol

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Crystal data

$C_{12}H_{12}O$
M_r = 172.22
Orthorhombic, $Pca2_1$
a = 9.8022 (6) Å
b = 14.9047 (9) Å
c = 12.6430 (7) Å
V = 1847.13 (19) Å^3
Z = 8
F(000) = 736
D_x = 1.239 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9816 reflections
θ = 3.5–78.7°
μ = 0.60 mm^{-1}
T = 173 K
Prism, colourless
0.59 × 0.44 × 0.22 mm

Data collection

Bruker PHOTON 100 CMOS diffractometer
Radiation source: sealed tube
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2014)
T_{min} = 0.776, T_{max} = 0.931
60021 measured reflections
3937 independent reflections
3893 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 78.9°, θ_{min} = 3.0°
h = −12→12
k = −18→18
l = −16→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.074
S = 1.04
3937 reflections
261 parameters
1 restraint
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0419P)^2 + 0.2448P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Absolute structure: Flack x determined using 1786 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.04 (3)

Special details

Experimental. *SADABS2014*/5 (Bruker,2014/5) was used for absorption correction. wR2(int) was 0.0570 before and 0.0501 after correction. The Ratio of minimum to maximum transmission is 0.8328. The λ/2 correction factor is 0.00150.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.49885 (12)	0.45896 (7)	0.36984 (11)	0.0337 (3)
H1	0.580 (3)	0.4703 (14)	0.3905 (19)	0.045 (6)*
C1	0.54796 (17)	0.21367 (11)	0.30591 (12)	0.0309 (3)
C2	0.45133 (19)	0.16711 (14)	0.25009 (14)	0.0406 (4)
H2	0.3956 (14)	0.2000 (8)	0.1943 (14)	0.049*
C3	0.4267 (3)	0.07555 (15)	0.26726 (17)	0.0538 (5)
H3	0.360 (2)	0.0452 (9)	0.2269 (12)	0.065*
C4	0.4994 (3)	0.03039 (13)	0.34271 (19)	0.0533 (5)
H4	0.4828 (5)	−0.0293 (17)	0.3542 (4)	0.064*
C5	0.5996 (2)	0.07497 (11)	0.40304 (15)	0.0397 (4)
C6	0.6740 (2)	0.03077 (14)	0.48406 (19)	0.0536 (5)
H6	0.6538 (6)	−0.0342 (17)	0.4997 (5)	0.064*
C7	0.7716 (2)	0.07348 (17)	0.54095 (18)	0.0575 (6)
H7	0.8239 (16)	0.0399 (10)	0.5981 (17)	0.069*
C8	0.8006 (2)	0.16422 (15)	0.52095 (16)	0.0482 (5)
H8	0.8739 (19)	0.1952 (8)	0.5620 (11)	0.058*
C9	0.72891 (17)	0.21065 (12)	0.44539 (13)	0.0346 (3)
H9	0.7492 (5)	0.2748 (14)	0.4332 (3)	0.042*
C10	0.62625 (17)	0.16800 (11)	0.38452 (12)	0.0312 (3)
C11	0.56252 (17)	0.31391 (11)	0.29043 (13)	0.0318 (3)
H11A	0.5286 (5)	0.3305 (3)	0.2212 (11)	0.038*
H11B	0.6580 (15)	0.3305 (3)	0.29433 (14)	0.038*
C12	0.48255 (17)	0.36354 (10)	0.37543 (14)	0.0334 (3)
H12A	0.3873 (16)	0.3491 (3)	0.36835 (17)	0.040*
H12B	0.5122 (5)	0.3431 (3)	0.4438 (11)	0.040*
O2	0.26483 (13)	0.54063 (8)	0.44908 (10)	0.0355 (3)
H2A	0.333 (3)	0.5135 (17)	0.424 (2)	0.051 (6)*
C21	0.21629 (15)	0.37666 (10)	0.58262 (12)	0.0281 (3)
C22	0.14186 (16)	0.33293 (11)	0.50662 (14)	0.0325 (3)
H22	0.0633 (18)	0.3629 (7)	0.4757 (7)	0.039*
C23	0.17591 (18)	0.24575 (11)	0.47191 (13)	0.0350 (4)
H23	0.1248 (13)	0.2184 (7)	0.4197 (13)	0.042*
C24	0.28412 (17)	0.20191 (10)	0.51537 (14)	0.0317 (3)
H24	0.3075 (5)	0.1431 (13)	0.4909 (6)	0.038*
C25	0.36234 (15)	0.24240 (10)	0.59631 (12)	0.0269 (3)
C26	0.47452 (17)	0.19757 (11)	0.64316 (13)	0.0325 (3)
H26	0.4950 (5)	0.1380 (14)	0.6223 (5)	0.039*
C27	0.55353 (18)	0.23832 (13)	0.71755 (13)	0.0367 (4)
H27	0.6345 (18)	0.2052 (8)	0.7494 (7)	0.044*
C28	0.52301 (17)	0.32634 (12)	0.75026 (13)	0.0341 (4)
H28	0.5807 (14)	0.3558 (7)	0.8037 (13)	0.041*
C29	0.41387 (16)	0.37134 (11)	0.70841 (12)	0.0297 (3)
H29	0.3933 (5)	0.4323 (13)	0.7331 (6)	0.036*
C30	0.33003 (15)	0.33137 (10)	0.63004 (11)	0.0255 (3)
C31	0.18036 (16)	0.47189 (11)	0.61290 (13)	0.0316 (3)

H31A	0.18674 (18)	0.47767 (14)	0.6894 (12)	0.038*
H31B	0.0860 (15)	0.4833 (2)	0.5930 (3)	0.038*
C32	0.27051 (17)	0.54330 (11)	0.56206 (14)	0.0332 (4)
H32A	0.2407 (5)	0.6039 (9)	0.5870 (4)	0.040*
H32B	0.3670 (15)	0.53414 (16)	0.5854 (4)	0.040*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0312 (6)	0.0279 (5)	0.0422 (6)	0.0007 (4)	0.0011 (5)	0.0058 (5)
C1	0.0316 (8)	0.0341 (8)	0.0269 (7)	0.0009 (6)	0.0062 (6)	−0.0008 (6)
C2	0.0405 (9)	0.0497 (10)	0.0316 (8)	−0.0042 (8)	−0.0002 (7)	−0.0046 (8)
C3	0.0626 (13)	0.0508 (11)	0.0481 (12)	−0.0178 (10)	0.0068 (10)	−0.0190 (9)
C4	0.0698 (13)	0.0313 (9)	0.0588 (13)	−0.0084 (9)	0.0208 (11)	−0.0102 (8)
C5	0.0457 (10)	0.0296 (8)	0.0439 (9)	0.0089 (7)	0.0158 (8)	0.0006 (7)
C6	0.0608 (13)	0.0387 (10)	0.0611 (13)	0.0213 (9)	0.0209 (11)	0.0127 (9)
C7	0.0501 (12)	0.0701 (14)	0.0523 (12)	0.0306 (11)	0.0102 (9)	0.0245 (11)
C8	0.0333 (9)	0.0717 (13)	0.0397 (10)	0.0109 (9)	0.0026 (8)	0.0093 (9)
C9	0.0306 (7)	0.0420 (9)	0.0312 (8)	0.0043 (7)	0.0051 (6)	0.0040 (7)
C10	0.0322 (7)	0.0322 (8)	0.0290 (8)	0.0043 (6)	0.0090 (6)	0.0002 (6)
C11	0.0308 (7)	0.0347 (8)	0.0298 (7)	0.0013 (6)	0.0025 (6)	0.0070 (6)
C12	0.0308 (8)	0.0292 (7)	0.0402 (8)	0.0000 (6)	0.0085 (7)	0.0060 (7)
O2	0.0316 (6)	0.0351 (6)	0.0396 (6)	0.0069 (5)	0.0010 (5)	0.0029 (5)
C21	0.0249 (7)	0.0311 (7)	0.0283 (7)	−0.0033 (6)	0.0054 (6)	0.0001 (6)
C22	0.0266 (7)	0.0375 (8)	0.0334 (8)	−0.0037 (6)	−0.0014 (6)	0.0023 (7)
C23	0.0360 (8)	0.0370 (8)	0.0320 (8)	−0.0125 (7)	−0.0024 (7)	−0.0040 (6)
C24	0.0361 (8)	0.0261 (7)	0.0330 (8)	−0.0077 (6)	0.0049 (7)	−0.0034 (6)
C25	0.0276 (7)	0.0277 (7)	0.0255 (7)	−0.0043 (6)	0.0055 (6)	0.0009 (5)
C26	0.0351 (8)	0.0301 (8)	0.0324 (8)	0.0029 (6)	0.0055 (6)	0.0010 (6)
C27	0.0308 (8)	0.0457 (9)	0.0337 (9)	0.0045 (7)	−0.0006 (7)	0.0061 (7)
C28	0.0304 (8)	0.0444 (9)	0.0274 (8)	−0.0026 (7)	−0.0014 (6)	−0.0020 (7)
C29	0.0308 (8)	0.0327 (8)	0.0256 (7)	−0.0035 (6)	0.0029 (6)	−0.0031 (6)
C30	0.0244 (6)	0.0276 (7)	0.0244 (7)	−0.0040 (5)	0.0046 (5)	0.0009 (5)
C31	0.0260 (7)	0.0340 (8)	0.0349 (8)	0.0041 (6)	0.0023 (6)	−0.0031 (6)
C32	0.0298 (8)	0.0304 (8)	0.0393 (9)	0.0026 (6)	−0.0014 (7)	−0.0023 (6)

Geometric parameters (Å, º)

O1—H1	0.86 (3)	O2—H2A	0.84 (3)
O1—C12	1.4330 (18)	O2—C32	1.430 (2)
C1—C2	1.370 (2)	C21—C22	1.371 (2)
C1—C10	1.428 (2)	C21—C30	1.435 (2)
C1—C11	1.514 (2)	C21—C31	1.512 (2)
C2—H2	1.02 (2)	C22—H22	0.97 (2)
C2—C3	1.403 (3)	C22—C23	1.411 (2)
C3—H3	0.94 (3)	C23—H23	0.92 (2)
C3—C4	1.367 (4)	C23—C24	1.362 (3)
C4—H4	0.92 (3)	C24—H24	0.96 (2)

C4—C5	1.410 (3)	C24—C25	1.414 (2)
C5—C6	1.420 (3)	C25—C26	1.417 (2)
C5—C10	1.430 (2)	C25—C30	1.428 (2)
C6—H6	1.01 (3)	C26—H26	0.95 (2)
C6—C7	1.356 (4)	C26—C27	1.361 (3)
C7—H7	1.02 (3)	C27—H27	1.02 (2)
C7—C8	1.405 (3)	C27—C28	1.408 (3)
C8—H8	1.00 (3)	C28—H28	0.98 (2)
C8—C9	1.373 (3)	C28—C29	1.369 (2)
C9—H9	0.99 (2)	C29—H29	0.98 (2)
C9—C10	1.417 (2)	C29—C30	1.418 (2)
C11—H11A	0.969 (15)	C31—H31A	0.973 (16)
C11—H11B	0.969 (15)	C31—H31B	0.973 (16)
C11—C12	1.522 (2)	C31—C32	1.525 (2)
C12—H12A	0.962 (15)	C32—H32A	1.001 (15)
C12—H12B	0.962 (15)	C32—H32B	1.001 (15)

C12—O1—H1	106.5 (15)	C32—O2—H2A	110.5 (17)
C2—C1—C10	119.24 (16)	C22—C21—C30	118.85 (14)
C2—C1—C11	119.91 (16)	C22—C21—C31	119.99 (14)
C10—C1—C11	120.65 (15)	C30—C21—C31	121.13 (14)
C1—C2—H2	118.9	C21—C22—H22	119.0
C1—C2—C3	122.13 (19)	C21—C22—C23	121.98 (15)
C3—C2—H2	118.9	C23—C22—H22	119.0
C2—C3—H3	120.1	C22—C23—H23	120.0
C4—C3—C2	119.8 (2)	C24—C23—C22	120.04 (15)
C4—C3—H3	120.1	C24—C23—H23	120.0
C3—C4—H4	119.7	C23—C24—H24	119.7
C3—C4—C5	120.54 (18)	C23—C24—C25	120.64 (14)
C5—C4—H4	119.7	C25—C24—H24	119.7
C4—C5—C6	121.98 (19)	C24—C25—C26	121.48 (15)
C4—C5—C10	119.70 (18)	C24—C25—C30	119.47 (14)
C6—C5—C10	118.30 (18)	C26—C25—C30	119.03 (14)
C5—C6—H6	119.1	C25—C26—H26	119.3
C7—C6—C5	121.84 (19)	C27—C26—C25	121.33 (15)
C7—C6—H6	119.1	C27—C26—H26	119.3
C6—C7—H7	120.0	C26—C27—H27	120.1
C6—C7—C8	119.94 (19)	C26—C27—C28	119.86 (16)
C8—C7—H7	120.0	C28—C27—H27	120.1
C7—C8—H8	119.8	C27—C28—H28	119.7
C9—C8—C7	120.5 (2)	C29—C28—C27	120.60 (16)
C9—C8—H8	119.8	C29—C28—H28	119.7
C8—C9—H9	119.5	C28—C29—H29	119.4
C8—C9—C10	120.99 (18)	C28—C29—C30	121.13 (15)
C10—C9—H9	119.5	C30—C29—H29	119.4
C1—C10—C5	118.54 (16)	C25—C30—C21	118.97 (14)
C9—C10—C1	123.06 (15)	C29—C30—C21	122.99 (14)
C9—C10—C5	118.40 (16)	C29—C30—C25	118.03 (14)

C1—C11—H11A	109.7	C21—C31—H31A	108.7
C1—C11—H11B	109.7	C21—C31—H31B	108.7
C1—C11—C12	109.87 (13)	C21—C31—C32	114.43 (13)
H11A—C11—H11B	108.2	H31A—C31—H31B	107.6
C12—C11—H11A	109.7	C32—C31—H31A	108.7
C12—C11—H11B	109.7	C32—C31—H31B	108.7
O1—C12—C11	112.96 (13)	O2—C32—C31	112.26 (14)
O1—C12—H12A	109.0	O2—C32—H32A	109.2
O1—C12—H12B	109.0	O2—C32—H32B	109.2
C11—C12—H12A	109.0	C31—C32—H32A	109.2
C11—C12—H12B	109.0	C31—C32—H32B	109.2
H12A—C12—H12B	107.8	H32A—C32—H32B	107.9

C1—C2—C3—C4	0.8 (3)	C21—C22—C23—C24	1.1 (2)
C1—C11—C12—O1	176.20 (13)	C21—C31—C32—O2	59.58 (17)
C2—C1—C10—C5	−0.7 (2)	C22—C21—C30—C25	0.2 (2)
C2—C1—C10—C9	179.51 (15)	C22—C21—C30—C29	179.33 (14)
C2—C1—C11—C12	95.94 (18)	C22—C21—C31—C32	−100.07 (17)
C2—C3—C4—C5	−0.4 (3)	C22—C23—C24—C25	0.8 (2)
C3—C4—C5—C6	178.1 (2)	C23—C24—C25—C26	179.43 (15)
C3—C4—C5—C10	−0.5 (3)	C23—C24—C25—C30	−2.2 (2)
C4—C5—C6—C7	179.09 (19)	C24—C25—C26—C27	176.88 (15)
C4—C5—C10—C1	1.1 (2)	C24—C25—C30—C21	1.6 (2)
C4—C5—C10—C9	−179.13 (16)	C24—C25—C30—C29	−177.53 (14)
C5—C6—C7—C8	0.6 (3)	C25—C26—C27—C28	0.9 (3)
C6—C5—C10—C1	−177.61 (16)	C26—C25—C30—C21	−179.92 (14)
C6—C5—C10—C9	2.2 (2)	C26—C25—C30—C29	0.9 (2)
C6—C7—C8—C9	1.2 (3)	C26—C27—C28—C29	0.4 (3)
C7—C8—C9—C10	−1.2 (3)	C27—C28—C29—C30	−1.0 (2)
C8—C9—C10—C1	179.27 (16)	C28—C29—C30—C21	−178.79 (14)
C8—C9—C10—C5	−0.5 (2)	C28—C29—C30—C25	0.3 (2)
C10—C1—C2—C3	−0.2 (3)	C30—C21—C22—C23	−1.6 (2)
C10—C1—C11—C12	−78.87 (18)	C30—C21—C31—C32	78.18 (18)
C10—C5—C6—C7	−2.2 (3)	C30—C25—C26—C27	−1.5 (2)
C11—C1—C2—C3	−175.10 (17)	C31—C21—C22—C23	176.68 (15)
C11—C1—C10—C5	174.12 (14)	C31—C21—C30—C25	−178.05 (13)
C11—C1—C10—C9	−5.6 (2)	C31—C21—C30—C29	1.1 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.86 (3)	1.96 (3)	2.7931 (17)	163 (2)
O2—H2*A*···O1	0.84 (3)	1.94 (3)	2.7834 (17)	176 (2)

Symmetry code: (i) *x*+1/2, −*y*+1, *z*.